

## Renormalization-Group Transformations on Quantum States

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We construct a general renormalization-group transformation on quantum states, independent of any Hamiltonian dynamics of the system. We illustrate this procedure for translational invariant matrix product states in one dimension and show that product, Greenberger-Horne-Zeilinger,  $W$ , and domain wall states are special cases of an emerging classification of the fixed points of this coarse-graining transformation.

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The renormalization group (RG) provides a procedure to obtain an effective long-distance description of a physical system. Following Wilson's seminal ideas [1], RG transformations are usually constructed in the space of Hamiltonians and are made of two distinct steps: first, a coarse-graining transformation is implemented to integrate out short-distance information, and, second, a rescaling of length scales and operators restores the original picture. This transformation is exact in the sense that long-distance observables remain unaltered, since they can be computed either with the original operators and Hamiltonian or with their renormalized counterparts to yield the same result. The exact RG transformation can be conveniently truncated so as to have a very powerful technique to retain only relevant long-distance degrees of freedom.

The success of RG is ubiquitous. Wilson's original idea has been modified to yield the density matrix renormalization-group (DMRG) [2] algorithm which optimizes the RG truncation, that is, the choice of relevant degrees of freedom to be retained. DMRG has been highly successful in describing the ground state properties in one-dimensional noncritical systems, and it can be understood as a variational method within the set of so-called matrix product states [3–5] discussed below.

From a quantum information (QI) perspective, renewed attention has been placed on quantum states. Many unexpected quantum state properties have been discovered and analyzed irrespectively of the dynamics that may produce them. It is then natural to review our understanding of RG focusing only on quantum states. This is actually the very origin of Kadanoff's classical block spin transformation [6], which has not been pursued on quantum states so far. The reason for the lack of a quantum coarse-graining analysis is related to the difficulty of parametrizing the Hilbert space of many-body systems as opposed to simple Hamiltonians and to the complexity of dealing with wave functions in quantum field theory.

Let us now introduce the general idea of the RG transformation on pure quantum states for  $m$ -site systems, where the local degrees of freedom correspond to a  $d$ -dimensional Hilbert space. In analogy with the standard

RG, we proceed in steps in which we (i) merge groups of neighboring sites into new ones and rescale the variables correspondingly, and (ii) identify states which are equivalent under local unitary operations. This identification is motivated by the fact that physics at long scales does not depend on the choice of local basis and, as it becomes clear below, gives rise to coarse graining and irreversibility. Technically, (ii) is realized by introducing an equivalence relation in Hilbert space, namely,  $\psi \cong \tilde{\psi}$  if there exist local unitaries  $U_1, \dots, U_m$  such that  $|\tilde{\psi}\rangle = U_1 \otimes \dots \otimes U_m |\psi\rangle$ . That is, two states are identified if they differ merely by a change in the local basis. Thus, the RG transformation in each step can be viewed as a map between the resulting equivalence classes  $\{\psi\} \xrightarrow{\text{RG}} \{\psi'\}$ . In practice, we perform the RG transformation on a representative which is conveniently selected after each step.

We describe now the above procedure in more detail for a 1D system with translational symmetry. Given a representative  $\psi$  of a class  $\{\psi\}$ , we determine a representative of the class  $\{\psi'\}$  in the next step as follows. We pairwise group the sites in the system and define a coarse-graining transformation for every pair of local basis states, e.g., for the sites  $2j$  and  $2j+1$ , as  $|p\rangle_{2j}|q\rangle_{2j+1} = |pq\rangle_j$ , where the indices  $p$  and  $q$  range from 1 to  $d$  and label the basis states in the original  $d$ -dimensional Hilbert spaces, whereas  $pq$  stands for its plain product and ranges from 1 to  $d^2$  labeling the natural product basis in the coarse Hilbert space. This still reversible transformation yields a state  $\psi'$ . Then we are allowed to take any new representative out of the equivalence class

$$\{|\psi'\rangle\} = \{U \otimes \dots \otimes U |\psi\rangle\}, \quad (1)$$

where a  $d^2 \times d^2$  unitary matrix  $U$  performs the change of representative in the coarse-grained space. Since this identification of states is a simple but crucial step in the transformation, we emphasize the following points.

(a) Identifying states which are equivalent under local unitary transformations makes the transformation irreversible unless we keep track of the unitaries applied in every

step. In this case the expectation values of all initial observables can be recovered exactly.

(b) The freedom to take a unitary transformation in the coarse-grained spaces goes beyond the freedom given by a product of unitary matrices in the original Hilbert spaces. The matrix  $U$  can be nonlocal as seen by the  $2j$  and  $2j + 1$  sites. Hence, local information about individual sites is washed out, while all the quantum correlations relating the coarse-grained block to other ones are preserved.

(c) The fact that we keep translational symmetry by taking all  $U_i = U$  assures that not only correlations on large scales but also global properties, which refer to a particular local basis (like the magnetization), survive the transformation.

To complete a RG transformation we simply need to rescale distances, i.e., to double the lattice spacing.

Exact RG transformations are often truncated in order to become of practical use. Let us, for example, consider the state after  $n$  coarse-graining steps, where each *local* site corresponds to  $2^n$  original spins. We are interested in describing long-range effects, hence in the degrees of freedom of the  $d^{2^n}$ -dimensional Hilbert space that couple to the outer sites (all the other information is local). In the case of ground states of 1D noncritical spin chains, for example, we know that the entropy of a block of spins saturates to a finite value, indicating that, indeed, very few degrees of freedom couple to the outer sites [7]. Mathematically, this means that there exists a local isometry  $U$  that transforms the  $d^{2^n}$ -dimensional space into a much smaller one, without practically affecting the correlations between the different blocks. The whole issue of truncation in RG then consists of coming up with an optimal algorithm for keeping the relevant degrees of freedom. Obviously, these relevant degrees of freedom will be exactly the ones that correspond to the largest weights in the reduced density operator of the block of  $2^n$  spins. This is very much related to the concept of the density operator in DMRG, although in that case only half-infinite blocks are considered.

In the following we explicitly carry out the RG transformations in terms of matrix product states (MPS). In this representation, the whole procedure can be naturally implemented, and the nature of the fixed points becomes transparent. Any 1D translationally invariant state can be written in its MPS form as [5]

$$|\psi\rangle = \sum_{p_1, p_2, \dots, p_m=1}^d \text{Tr}(A^{p_1} A^{p_2} \dots A^{p_m}) |p_1, p_2, \dots, p_m\rangle, \quad (2)$$

where the  $D \times D$  matrices  $\{A^p\}$  parametrize the state. The value of the dimension  $D \leq d^{m/2}$  depends on the particular state [8]; however, the success of DMRG shows that in practice small  $D$ 's typically yield very good approximations [3].

The quantum coarse-graining procedure where we map two neighboring spins to one new block spin can now be fully characterized in terms of the matrices  $\{A^p\}$ . Clearly,

merging neighboring sites, say  $i$  and  $i + 1$ , means merging the respective matrices  $A^{p_i}$  and  $A^{p_{i+1}}$  to a larger set of new  $D \times D$  matrices of the form  $\tilde{A}_{(\alpha\gamma)}^{(pq)} := \sum_{\beta=1}^D A_{\alpha\beta}^p A_{\beta\gamma}^q$ . For the second step in the transformation, the selection of a convenient representative for the equivalence class, we start from the singular value decomposition

$$\tilde{A}_{(\alpha\gamma)}^{(pq)} = \sum_{l=1}^{\min(d^2, D^2)} U_l^{\dagger(pq)} \lambda^l V_{(\alpha\gamma)}^l, \quad (3)$$

where  $(pq)$  and  $(\alpha\gamma)$  are understood as combined indices. Note that  $U$  in Eq. (3) corresponds to a local unitary in the coarse-grained space. By considering equivalence classes we can thus disregard this change of local basis and select a new representative characterized by matrices  $A^l$  so that

$$A^p \xrightarrow{\text{RG}} A^l = \lambda^l V^l. \quad (4)$$

The advantage of this representative is that the Hilbert space corresponding to the block spins remains bounded above by  $D^2$  at any step, as it is clear from the singular value decomposition. That is, Eq. (3) shows us what the relevant degrees of freedom are, and the consideration of equivalence classes allows us to discard the irrelevant ones. In this way it is possible to perform an exact coarse graining on finite dimensional matrix product states without any need of truncation.

Before introducing a formalism to characterize the fixed points of this exact renormalization flow, let us present some simple examples. The first one is provided by product states (for which  $D = 1$ ,  $A^1 = 1$ , and  $A^k = 0$  for  $k = 2, \dots, d$  and  $A^i = A^i$ ). These are precisely the states obtained for massive theories in their infrared fixed points. A significant further example corresponds to Greenberger-Horne-Zeilinger (GHZ)-like states [9]. If we take  $d = 2$  and  $A^0 = |0\rangle\langle 0|$ ,  $A^1 = |1\rangle\langle 1|$  the RG transformation reads  $A^i \xrightarrow{\text{RG}} A^i = A^i$ . Those states, indeed, appear as RG infrared points in, e.g., the quantum Ising chain for vanishing external magnetic field [10].

Let us now construct a general formalism by which the fixed points of the RG flow can be characterized. In order to circumvent the arbitrariness in the choice of the local bases, we introduce the auxiliary  $D^2 \times D^2$  transfer matrix

$$E = \sum_{p=1}^D A^p \otimes \bar{A}^p, \quad (5)$$

where the bar indicates complex conjugation. Note that if we change the local basis by choosing  $\tilde{A}^q = \sum_p U_p^q A^p$  with  $U$  unitary, we have

$$\tilde{E} = \sum_{q=1}^D \tilde{A}^q \otimes \bar{\tilde{A}}^q = \sum_{p=1}^D A^p \otimes \bar{A}^p = E. \quad (6)$$

Conversely, the matrix  $E$  uniquely defines the matrices  $A^p$  up to such a local unitary operator, and thus it parametrizes

the equivalence class of  $D$ -dimensional MPS where all elements of the class are related by local unitary operations [11]. Furthermore, a RG step corresponds to the simple transformation  $E \xrightarrow{\text{RG}} E' = E^2$ . Therefore, in order to study the alluded fixed points, we just have to characterize the class of possible operators  $\{E_\infty\} = \{\lim_{n \rightarrow \infty} E^n\}$  for some  $E$  in the form (5). Since we can always choose the largest eigenvalue of  $E$  to be equal to 1 [12], we just have to characterize all matrices  $E$  of the form (5) that have only eigenvalues of magnitude 1 or 0 (eigenvalues smaller than 1 will decay exponentially along repeated coarse-graining steps).

In the generic case, the largest eigenvalue of  $E$  will be nondegenerate and both its left and right eigenvectors will have a maximal Schmidt rank; that is,  $E^\infty = |\Phi_R\rangle\langle\Phi_L|$ , where the reduced density operators of  $\Phi_{L,R}$  are rank  $D$  matrices. With the similarity transformation [12] we can always choose  $|\Phi_R\rangle = \sum_{i=1}^D |ii\rangle$  and  $|\Phi_L\rangle = \sum_{i=1}^D \lambda_i |ii\rangle$ , with  $\lambda_i > 0$ . From these eigenvectors we can directly read off the matrices  $A^{(pq)} = \sqrt{\lambda_q} |p\rangle\langle q|$  with  $p, q = 1, \dots, D$ . Thus, at the fixed point, the scale-invariant state (representative of the equivalence class) can be written in terms of two auxiliary spins at each point, which are in an entangled state  $|\Phi_L\rangle$  with its neighbors. This conclusion is very appealing, and has the following consequences.

All connected correlation functions of the form  $\langle O^i O^j \rangle - \langle O^i \rangle \langle O^j \rangle$  are exactly zero when  $j > i + 1$ ; this is exactly what one expects from a generic state by looking at it in a coarse-grained way: the correlations decay exponentially along the renormalization flow and become zero at the fixed point.

In terms of the picture introduced in [8], coarse-graining turns the virtual underlying spins into real ones but changes the maximally entangled states into  $|\Phi_R\rangle$ .

The entropy of a block of spins of length  $L$  is independent of  $L$  and is exactly twice the entropy of entanglement of  $|\Phi_R\rangle$ .

In fact, the entropy of a block of  $L$  spins, i.e., their entanglement with the rest of the chain, increases monotonically by coarse graining if we do not rescale the lengths. By the strong subadditivity of the entropy (cf. [13]) this is even true in general for all translationally invariant states.

As an illustration of the generic case analyzed above, let us consider the ground state of the Affleck-Kennedy-Lieb-Tasaki Hamiltonian [4], for which  $A^p = \sigma^p$  ( $p = 1, \dots, 3$ ) are the Pauli matrices. Some simple algebra shows that  $E$  has eigenvalues 3, 1, -1, -1 and hence no degeneracy in the largest eigenvalue. The fixed point is given by the eigenvector corresponding to eigenvalue 3, namely,  $E_i = |I\rangle\langle I|$  with  $|I\rangle = \sum_{i=1}^2 |ii\rangle$ . Hence, it is a dimer of maximally entangled states, i.e., in the language of QI a perfect resource for a quantum repeater. Intriguingly, this is also the exact fixed point of the 1D cluster state [14] represented by  $A^0 = |0\rangle\langle 0| + |1\rangle\langle 1|$ ,  $A^1 = |1\rangle\langle 0| - |0\rangle\langle 1|$ . However, in

this case the fixed point is already obtained after one coarse-graining step as the corresponding  $E$  contains a nilpotent Jordan block:

$$E = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \quad E_{cl}^2 = \sum_{ij} |ii\rangle\langle jj|. \quad (7)$$

The formalism developed above can also be applied in the case  $D \rightarrow \infty$ . To illustrate that, let us consider an Ising chain with transverse magnetic field or an anisotropic Heisenberg antiferromagnet. In the noncritical regime, their correlation length  $\xi$  is finite, which implies that the associated operator  $E$  will have a nondegenerate largest eigenvalue [ $1/\xi \propto \ln(\lambda_1/\lambda_2)$ ]. Accordingly, the fixed point of the coarse-graining map will therefore consist of a dimer state. The eigenvalues of the reduced density operator of a half-infinite chain are precisely the Schmidt coefficients of the bipartite states making up the dimer. We can, in fact, determine these coefficients by using the results of Peschel, Kaulke, and Legeza [15], who have been able to determine the mentioned reduced density operator exactly. For the Ising model we have

$$\lambda_{(n_1, n_2, \dots, n_\infty)} = \begin{cases} e^{-\epsilon \sum_{j=0}^{\infty} (2j+1)n_j}, & \lambda < 1, \\ e^{-\epsilon \sum_{j=0}^{\infty} 2jn_j}, & \lambda > 1. \end{cases} \quad (8)$$

Here  $\epsilon = \pi K[(1 - \mu^2)^{1/2}]/K(\mu)$ , with  $K$  the complete elliptic integral of the first kind,  $\mu = \min(\lambda, 1/\lambda)$ , and  $n_j \in \{0, 1\}$ . In the case of the noncritical Heisenberg model  $H_{XXZ} = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^z \sigma_{i+1}^z + \Delta \sigma_i^z \sigma_{i+1}^z$  with  $\Delta > 1$ , the eigenvalues are as in the Ising case with  $\lambda > 1$ , but with  $\epsilon = \text{arccosh}(\Delta)$ .

We consider now the full classification of fixed points for the simplest nontrivial case  $D = 2$ . By considering the right eigenvectors of  $E$  corresponding to the maximal eigenvalue, we have two possibilities [16]: (a) one of them, say  $|\Phi_R\rangle$ , is entangled, and (b) there exists only one eigenvector which corresponds to a product state.

In the first case (a), by using the similarity transformation [11] we can always take  $|\Phi_R\rangle = \sum_{i=1}^2 |ii\rangle$ . Using the isomorphism [16] and the full classification of trace preserving completely positive maps acting on a qubit [17], one can prove that  $E_\infty$  has rank 1, 4, or 2. For the first cases, we recover the generic case studied above or obtain a product state, respectively. When the rank is 2, we obtain  $A^0 = |0\rangle\langle 00|$ ;  $A^1 = |1\rangle\langle 11|$ , i.e., the GHZ state [9] studied above.

The situation is more complicated in the second case (b), as this implies that  $E$  is not diagonalizable but has a Jordan-block decomposition. Some tedious but straightforward algebra leads to two different possibilities for the fixed points. In the first case the effective Hilbert space is two dimensional and

$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & \exp(-i\theta) \end{pmatrix}, \quad A^1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (9)$$

Note that  $A^0 A^1 = e^{-i\theta} A^1$  and that  $A^1$  is nilpotent; this immediately implies that the state, when written in the computational basis, consists of terms like  $|00 \cdots 010 \cdots 0\rangle$  where at most one  $|1\rangle$  appears. When  $\theta = 0$ , we recover the well-known  $W$  state [18], which is, indeed, scale invariant. In the second case of Jordan fixed points, the spins have effective support on a Hilbert space of dimension 3 [but 2 when  $\cos(\alpha) = 1$ ], and a possible decomposition is given by

$$A^0 = \begin{pmatrix} 0 & 0 \\ \cos(\alpha) \sin(\beta) & e^{i\theta} \end{pmatrix}, \quad A^1 = \begin{pmatrix} 0 & 0 \\ \sin(\alpha) & 0 \end{pmatrix}, \\ A^2 = \begin{pmatrix} e^{-i\theta} & 0 \\ \cos(\alpha) \cos(\beta) & 0 \end{pmatrix}. \quad (10)$$

As  $A^0 A^1 \propto A^1$ ,  $A^1 A^2 \propto A^2$ ,  $A^0 A^2 \propto A^1$ ,  $A^1 A^0 = 0$ ,  $A^2 A^1 = 0$ ,  $A^2 A^0 = 0$ , the state will be a superposition of terms of the form  $|00 \cdots 0122 \cdots 2\rangle$ . Therefore these scale-invariant states represent a linear combination of domain walls.

For the case  $D = 2$  this completes the classification of all fixed points, which remarkably correspond to almost all well-studied multipartite states encountered in QI. We note that in the thermodynamic limit case (b) in the classification is redundant in the sense that  $W$  and product state as well as domain wall and GHZ state become then locally indistinguishable. A distinction can, however, be relevant from a QI perspective, where it is more natural to carry out only a finite number of coarse-graining steps which enlarge the region of local accessibility only to a physically reasonable vicinity. In this context the system to be transformed can thus be finite.

For  $D > 2$  a coarse classification of the fixed points can be given by their possible decompositions into ergodic states and their periodic components discussed in [5].

Our work can be understood as a real space regulated approach to the renormalization of states in quantum field theories. We have concentrated here on 1D systems, since in that case MPS give a very useful description. Fortunately, the analogue of MPS in higher dimensions has been recently put forward [19], which may allow us to extend the analysis introduced here to two and three spatial dimensions. The case of critical chains, and more generally conformal field theories, requires also further work since the fact that entanglement scales logarithmically as the size of the system increases implies that the dimensionality of the coarse-grained Hilbert spaces will keep growing indefinitely.

Let us conclude with a comment on the irreversibility of RG flows. Our RG transformation defined on finite matrix product states incorporates unitarity in a natural way at variance with other approaches. Moreover, the eigenvalues

of  $E^2$  are smaller than the ones of  $E$ . RG flows will inevitably eliminate all the eigenvalues smaller than 1, which can be phrased as irrelevant pieces of the state. A careful treatment of the irreversibility of RG flows should incorporate the infinite dimensional case, associated with conformal field theories, and the discussion of degeneracy in the final relevant Hilbert space.

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